

U.S. PATENT DOCUMENTS

5,860,957	A	1/1999	Jacobsen et al.
5,900,252	A	5/1999	Calanchi et al.
5,948,433	A	9/1999	Burton et al.
5,972,366	A	10/1999	Haynes et al.
5,983,134	A	11/1999	Ostrow
5,985,307	A	11/1999	Hanson et al.
5,985,317	A	11/1999	Venkateshwaran et al.
6,004,534	A	12/1999	Langer et al.
6,010,715	A	1/2000	Wick et al.
6,024,975	A	2/2000	D'Angelo et al.
6,039,975	A	3/2000	Shah et al.
6,048,736	A	4/2000	Kosak
6,060,082	A	5/2000	Chen et al.
6,071,495	A	6/2000	Unger et al.
6,120,751	A	9/2000	Unger
6,131,570	A	10/2000	Schuster et al.
6,139,865	A	10/2000	Friend et al.
6,167,301	A	12/2000	Flower et al.
6,253,872	B1	7/2001	Neumann
6,256,533	B1	7/2001	Yuzhakov et al.
6,261,595	B1	7/2001	Stanley et al.
6,267,983	B1	7/2001	Fujii et al.
6,271,359	B1	8/2001	Norris et al.
6,274,552	B1	8/2001	Tamarkin et al.
6,316,652	B1	11/2001	Steliou

OTHER PUBLICATIONS

Berendsen et al., "Molecular dynamics with coupling to an external bath," *J Chem Phys.*, 1984, 81:3684-3690.

Darden et al., "Particle Mesh Ewald-an N.Log(N) method for Ewald sums in large systems," *J Chem Phys.*, 1993, 98:10089-10092.

Ekstrom et al., "Structure of HI-6*sarin-acetylcholinesterase determined by X-ray crystallography and molecular dynamics simulation: reactivator mechanism and design," *PLoS One*, 2009, 4(6):e5957, 19 pages.

Hornak et al., "Comparison of multiple Amber force fields and development of improved protein backbone parameters," *Proteins*, 2006, 65:712-725.

IUPAC-IUB Commission on Biochemical Nomenclature: Abbreviated Nomenclature of Synthetic Polypeptides (Polymerized Amino Acids), *Biochem.*, 1972, 11(5):942-944.

Jorgensen et al., "Comparison of simple potential functions for simulating liquid water," *J Chem Phys.*, 1983, 79:926-935.

Nishibata et al., "Confirmation of usefulness of a structure construction program based on three-dimensional receptor structure for rational lead generation," *J. Med. Chem.*, 1993, 36(20):2921-2928.

Nogarty, *Medicinal Chemistry A Biochemical Approach* (New York, Oxford University Press, 1985), pp. 388-392.

Oelschlaeger et al., "Modeling Domino Effects in Enzymes: Molecular Basis of the Substrate Specificity of the Bacterial Metallo- β -lactamases IMP-1 and IMP-6," *J. Biochemistry*, 2003, 42:8945-8956.

Oelschlaeger et al., "Insight into the mechanism of the IMP-1 metallo- β -lactamase by molecular dynamics simulations," *J. Protein Eng.*, 2003, 16:341-350.

Pang et al., "Computational and Experimental Studies of (2,2)-Bis(indo 1-1-yl-methyl)acetate Suggest the Importance of the Hydrophobic Effect in Aromatic Stacking Interactions," *J. Am. Chem. Soc.*, 1999, 121:1717-1725.

Pang, "Novel zinc protein molecular dynamics simulations: Steps toward antiangiogenesis for cancer treatment," *J. Mol. Model.*, 1999, 5:196-202.

Pang, "Three-dimensional model of a substrate-bound SARS chymotrypsin-like cysteine proteinase predicted by multiple molecular dynamics simulations: catalytic efficiency regulated by substrate binding," *Proteins*, 2004:57:747-757.

Pang, "Successful molecular dynamics simulation of two zinc complexes bridged by a hydroxide in phosphotriesterase using the cationic dummy atom method," *Proteins*, 2001, 45(3):183-189.

Pang et al., "Successful molecular dynamics simulation of the zinc-bound farnesyltransferase using the cationic dummy atom approach," *Protein Sci.*, 2000, 9(10):1857-1865.

Park et al., "Serotype-selective, small-molecule inhibitors of the zinc endopeptidase of botulinum neurotoxin serotype A," *Bioorg Med Chem.*, 2006, 14:395-408.

Pearlman et al., "AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules," *Comput Phys Commun.*, 1995, 91:1-41.

Schmidt and Stafford, "Fluorigenic substrates for the protease activities of botulinum neurotoxins serotypes A, B, and F," *Appl Environ Microbiol.*, 2003, 69:297-303.

Schmidt and Bostian, "Endoproteinase activity of type A botulinum neurotoxin: substrate requirements and activation by serum albumin," *J. Protein Chem.*, 1997, 16:19-26.

Segel, *Enzyme Kinetics* (New York, Wiley and Sons, 1975), pp. 170-178.

Shao et al., "Clustering molecular dynamics trajectories: I. Characterizing the performance of different clustering algorithms," *J Chem Theory Comput.*, 2007, 3:2312-2334.

Silvaggi et al., "Catalytic Features of the Botulinum Neurotoxin A Light Chain Revealed by High Resolution Structure of an Inhibitory Peptide Complex," *Biochemistry*, 2008, 47:5736-5745.

Tang et al., "Computer-aided lead optimization: improved small-molecule inhibitor of the zinc endopeptidase of botulinum neurotoxin serotype a," *PLoS One*, 2007, 8:e761, 8 pages.

* cited by examiner